

Claims

- [c1] 1.A method to conduct an experiment, comprising steps of:
selecting factors for the experiment;
estimating interactions among levels of the factors
assigning a probability value of positive interactions for each of the
estimated interactions;
effecting a combinatorial high throughput screening (CHTS) method on an
experimental space representing the levels; and
adjusting the probabilities for each interaction according to results of the
CHTS method.
- [c2] 2.The method of claim 1, comprising assigning a high probability value,
medium probability value or low probability value of each positive interaction
for each of the estimated interactions is assigned by a client or investigator.
- [c3] 3.The method of claim 1, wherein a high probability value, medium
probability value or low probability value of each positive interaction for each
of the estimated interactions.
- [c4] 4.The method of claim 1, wherein an investigator and a client who benefits
from results from the CHTS experiment in concert determine a probability
value to be assigned.
- [c5] 5.The method of claim 1, comprising assigning values to represent a high
probability value, medium probability value and low probability value of each
positive interaction for each of the estimated interactions.
- [c6] 6.The method of claim 1, comprising assigning 0.6 to about 0.99 value as a
high probability value, about 0.2 to about 0.59 value as a medium
probability value and about 0.01 to about 0.19 value as a low probability
value.
- [c7] 7.The method of claim 1, comprising assigning 0.7 to about 0.9 value as a
high probability value, about 0.2 to about 0.5 value as a medium probability
value and about .05 to about 0.15 value as a low probability value.

- [c8] 8.The method of claim 1, further comprising repeating a CHTS method step and an adjusting probabilities step until a best set of levels is selected.
- [c9] 9.The method of claim 1, comprising constructing an adjustable definitional model to represent the estimated interactions and assigned probabilities.
- [c10] *Sub* 10.The method of claim 1, wherein the model is a visual organizational aid.
- [c11] *M* 11.The method of claim 1, wherein the model is a virtual construct resident in a computer database.
- [c12] 12.The method of claim 1, wherein the CHTS method comprises defining a first experimental space by structuring the levels according to a Latin Square strategy.
- [c13] 13The method of claim 1, wherein the CHTS experiment comprises steps of; preparing a plurality of reagent compositions; formulating a combinatorial library of reactants from said plurality of reagent compositions; effecting parallel reaction of the library to produce products; and evaluating the products to select a lead from the library of reactants.
- [c14] 14.The method of claim 1, wherein conducting the CHTS experiment comprises providing a reactor plate comprising a substrate with an array of reaction cells containing at least one reactant according to an input factor level and reacting the reactant in parallel with other reactants.
- [c15] 15.The method of claim 1, wherein the CHTS comprises effecting parallel chemical reactions of an array of reactants defined as the experimental space.
- [c16] 16.The method of claim 1, wherein the CHTS comprises effecting parallel chemical reactions on a micro scale on reactants defined as the experimental space.
- [c17] 17.The method of claim 1, wherein the CHTS comprises an iteration of steps

of simultaneously reacting a multiplicity of tagged reactants and identifying a multiplicity of tagged products of the reaction and evaluating the identified products after completion of a single or repeated iteration.

- [c18] 18.The method of claim 1, wherein the experimental space factors comprise reactants, catalysts and conditions and the CHTS comprises
(A)(a) reacting a reactant selected from the experimental space under a selected set of catalysts or reaction conditions; and (b) evaluating a set of results of the reacting step; and
(B) reiterating step (A) wherein a selected experimental space selected for a step (a) is chosen as a result of an evaluating step (b) of a preceding iteration of step (A).
- [c19] 19.The method of claim 16, wherein the evaluating step (b) comprises identifying relationships between factor levels of the candidate chemical reaction space; and determining the chemical experimental space according to a full factorial design for the next iteration.
- [c20] 20.The method of claim 16, comprising reiterating (A) until a best set of factor levels of the chemical experimental space is selected.
- [c21] 21.The method of claim 1, wherein the factors include a catalyst system comprising a Group VIII B metal.
- [c22] 22.The method of claim 1, wherein the factors include a catalyst system comprising palladium.
- [c23] 23.The method of claim 1, wherein the factors include a catalyst system comprising a halide composition.
- [c24] 24.The method of claim 1, wherein the factors include an inorganic co-catalyst.
- [c25] 25.The method of claim 1, wherein the factors include a catalyst system includes a combination of inorganic co-catalysts.

[c26] 26.The method of claim 1, wherein the factors comprise a reactant or catalyst at least partially embodied in a liquid and effecting the CHTS method comprises contacting the reactant or catalyst with an additional reactant at least partially embodied in a gas, wherein the liquid forms a film having a thickness sufficient to allow a reaction rate that is essentially independent of a mass transfer rate of additional reactant into the liquid to synthesize products that comprise the results.

[c27] 27.A system for conducting an experiment, comprising;
a reactor for effecting a CHTS method on an experimental space to produce results; and
a programmed controller that stores an assigned probability value for estimated positive interactions between levels of factors of the experimental space and adjusts the probabilities for each interaction according to results of the CHTS method.

[c28] 28.The system of claim 27, wherein the assigned probability value is about 0.6 to about 0.99 value as a high probability value, about 0.2 to about 0.59 value as a medium probability value or about 0.01 to about 0.19 value as a low probability value.

[c29] 29.The system of claim 27, wherein the assigned probability value is about 0.7 to about 0.9 value as a high probability value, about 0.2 to about 0.5 value as a medium probability value or about .05 to about 0.15 value as a low probability value.

[c30] 30.The system of claim 27, wherein said defines a second experimental space according to the adjusted interaction probabilities.

[c31] 31.The system of claim 27, wherein the controller is a computer, processor or microprocessor.

[c32] 32.The system of claim 27, further comprising a dispensing assembly to charge factor levels of reactants or catalysts representing the catalyzed chemical experimental space to wells of an array plate for charging to the

reactor.

- [c33] 33.The system of claim 27, wherein the dispensing assembly is controlled by the controller to charge factor levels of reactants or catalysts according to the controller defined space.
- [c34] 34.The system of claim 27, further comprising a detector to detect results of the CHTS method effected in the reactor.

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